1-Aminocyclopentanecarboxylic acid, N-(neopentyloxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C17H31NO4/c1-5-6-9-12-21-14(19)17(10-7-8-11-17)18-15(20)22-13-16(2,3)4/h

InchiKey: NGENUFGXFKJHSV-UHFFFAOYSA-N

Formula: C17H31NO4

SMILES: CCCCCOC(=O)C1(N=C(O)OCC(C)(C)C)CCCC1

Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
hf	-784.06	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.009		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
tb	868.10	K	Joback Method
tc	1075.39	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392516&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature